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ENDF/B-VIIIrc1 ^{239}Pu Uncertainties: Constraints, Sampling, and Calibration to Jezebel

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Introduction

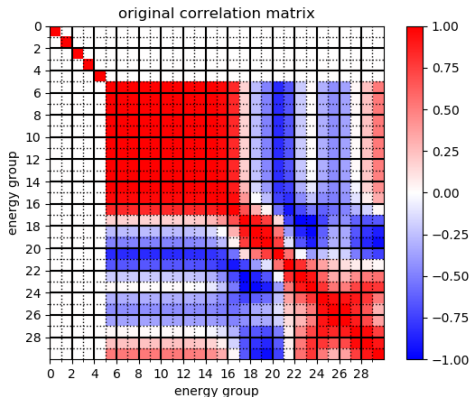
- The Goal:
 - We want to know the effect of nuclear-data uncertainties on the results of our physics simulations.
- We start from the uncertainties and correlations (covariances) provided by ENDF/B-VIIIrc1.
- We then fit to Jezebel.
- Details:
 - ^{239}Pu neutron cross sections, prompt fission neutron spectrum (χ -vector), and $\bar{\nu}$.
 - Reduced to 30 energy groups, numbered from low to high energy, using NJOY.
 - Cross sections for 6 reactions plus total cross section for each group
 - The order is: total, elastic, inelastic, n2n, n3n, fission, capture (mt1, mt2, mt4, mt16, mt17, mt18, mt102).
 - Thus, 270 nuclear data overall
 - All data are in single precision.

Constraints

- All sampled values must be non-negative (an inequality constraint)
 - Normally imposed either by discarding samples with negative values or doing lognormal sampling
- Sampled values must satisfy certain equality constraints.
 - For each energy group, the total cross section must be the sum of the cross sections of the individual reactions.
 - The sum of the values of the PFNS must be 1.
 - These equality constraints are linear and so may be imposed with proper specification of correlations.
 - However, as we will show, imposing equality constraints with correlations conflicts with lognormal sampling.
- Covariance matrices must be non-negative definite (all eigenvalues ≥ 0).
 - The covariance matrices that obey linear constraints are singular, thus have zero eigenvalues.
 - Due to finite precision arithmetic, some of these zero eigenvalues will appear to be negative but (hopefully) small.
 - How small is small enough?

A Correlation Matrix with Constraints

- This is the correlation matrix for the PFNS.
- The lowest five energy groups have zero variance.
- The large block of ones (red) locks the mid-range values together.
- The ones and near-ones close to the diagonal throughout maintain smoothness.
- The minus-one values (blue) impose the summation constraint by anticorrelating the high values with the mid-range.



Numerics

- The data are specified in single precision.
- The logarithmic range in the mean vectors and variances for both cross sections and PFNS is very large.
 - Up to 10^{12}
- The sensitivities of outputs of interest to input values obviously differ enormously.
 - Especially between cross sections for different reactions but also across energies
 - For example, fission versus n2n
 - Just because a quantity is small relative to others does not mean that it is not important.
- Sampling from the specified means and covariances requires spectral factorization of the covariance matrix, which operates globally over the entire matrix, so care must be taken that the large values do not wash out the (potentially important) small ones.

Fixing the Grouped Data to Satisfy The Constraints

- The grouped nuclear data, especially the covariance matrices, do not obey the constraints very well.
 - Never better than single precision (10^7), sometimes much worse.
 - The logarithmic range is much larger than this, up to 10^{12} with the current dataset.
- We should fix the covariance matrices (and possibly the mean vectors) to obey the constraints down to double precision.
- We need to impose constraints on a covariance matrix, Σ , in a particular order so that imposing one constraint is not undone by later fixes.
 1. Remove zero rows and columns
 2. Impose the equality constraints
 3. Perform the spectral factorization, $U\Lambda U^T = \Sigma$, where U is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues.
 4. Set all negative eigenvalues to zero
 5. Invert the spectral factorization

Imposing Linear Constraints on a Covariance Matrix

- The requirement:
 - A sample, s , must obey a set of linear constraints of the form $s \cdot C_i = k_i$ where C_i is the vector that defines the i -th constraint and k_i is an associated constant.
- Consequences:
 - The mean vector must satisfy the same constraints.
 - The covariance matrix must satisfy a set of constraints of the form $\Sigma C = 0$ where C is the matrix of the column vectors C_i .
- We impose the constraints by using projection operators. This is intended to minimize changes to the matrix and appears to do so. It is appropriate when the matrix is not too far from obeying the constraints. In worse cases, it may not be appropriate.

Imposing Constraints Using Projection Operators

- Scale Σ so that all variances are 1 by dividing each row and column by the square root of its diagonal element (the standard deviation).
 - Yes, this is the correlation matrix, but that is not what we are using it for.
 - Doing this eliminates problems of large logarithmic range and reduces problems of very different sensitivities.
- Scale the columns of C by dividing each component by its standard deviation.
- Orthonormalize the columns of C (using the QR decomposition),

$$\hat{C} = Q, \quad Q, R = QR(C). \quad (1)$$

- Compute $P_{\mathcal{C}_\perp}$, the operator that projects orthogonally onto the space that is orthogonal to the columns of C (and \hat{C}),

$$P_{\mathcal{C}_\perp} = I - \hat{C}\hat{C}^T. \quad (2)$$

- Compute Σ' , which obeys the constraints,

$$\Sigma' = P_{\mathcal{C}_\perp} \Sigma P_{\mathcal{C}_\perp}. \quad (3)$$

- Undo the scaling of Σ' by multiplying each row and column by its standard deviation.

What About Negative Values?

- About 7% of cross-section samples have at least one negative value.
- We choose to discard these samples.
- We found that about 6% of PFNS samples have at least one negative value.
- Because discarding 13% of samples seemed excessive, we elected to implement (multivariate) lognormal sampling for the PFNS.
 - The PFNS has only a single constraint versus 30 for the cross sections.
- It turns out that you cannot do multivariate lognormal sampling for a quantity with hard correlations (1 or -1 or values close to those).
 - “Transformation of correlation coefficients between normal and lognormal distribution and implications for nuclear applications”; Gašper Žerovnik, Andrej Trkov, Donald L. Smith, Roberto Capote; *Nuclear Instruments and Methods in Physics Research A* 727 (2013) 33–39
 - “Random Sampling of Correlated Parameters—a Consistent Solution for Unfavourable Conditions”; G. Žerovnik. A. Trkov. I. A. Kodeli, R. Capote, D. L. Smith; *Nuclear Data Sheets* 123 (2015) 185–190
- We have implemented a work-around that works well for our application.

Multivariate Lognormal Sampling

- A multivariate random variable Y has a lognormal distribution iff:

$$Y \equiv \exp(X), \quad X \sim N(\mu, \Sigma). \quad (4)$$

where \exp just means component-wise exponentiation.

- The mean and covariance matrix of Y are given by:

$$E[Y]_i = \exp \left[\mu_i + \frac{1}{2} \Sigma_{ii} \right] \quad (5)$$

$$\text{Cov}[Y]_{ij} = \exp \left[\mu_i + \mu_j + \frac{1}{2} (\Sigma_{ii} + \Sigma_{jj}) \right] (\exp(\Sigma_{ij}) - 1). \quad (6)$$

- We are given $E[Y]$ and $\text{Cov}[Y]$ so we want to invert Equations 5 and 6 to obtain μ and Σ .
- Even though these are transcendental equations, they can actually be inverted analytically.

Multivariate Lognormal Sampling (continued)

$$\mu_i = \log(E[Y]_i) - \frac{1}{2} \log \left(\frac{\text{Cov}[Y]_{ii}}{E[Y]_i^2} + 1 \right) \quad (7)$$

$$\Sigma_{ij} = \log \left(\frac{\text{Cov}[Y]_{ij}}{E[Y]_i E[Y]_j} + 1 \right). \quad (8)$$

- μ_i depends only on $E[Y]_i$ and $\text{Cov}[Y]_{ii}$.
- Σ_{ii} depends only on $E[Y]_i$ and $\text{Cov}[Y]_{ii}$.
- μ_i and Σ_{ii} are exactly the same as if each component were just an independent lognormal random variable.
- Σ_{ij} depends only on $E[Y]_i$, $E[Y]_j$, and $\text{Cov}[Y]_{ij}$.
- There is no guarantee that Σ as defined by Equation 8 will be a valid covariance matrix and it is easy to come up with cases where it will not be.
 - For example, a correlation of -1 and sufficiently large relative standard deviations for the two components will do it.
 - So will a correlation of 1 under certain circumstances.

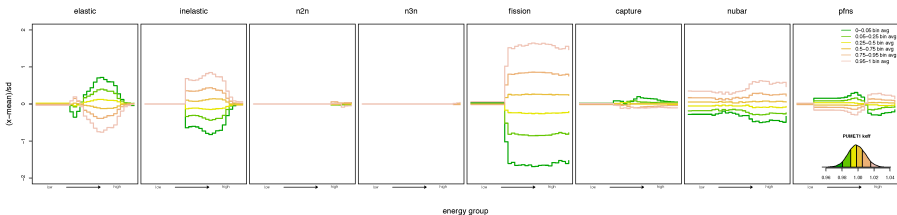
Multivariate Lognormal Sampling with Hard Correlations

1. Fix the covariance matrix, $\text{Cov}[Y]$, and mean vector, $E[Y]$, as appropriate.
 2. Remove zero rows and columns from the covariance matrix and corresponding components from the mean vector.
 3. Compute μ and the diagonal elements of Σ from Equations 7 and 8.
 4. Compute the correlation matrix, $\text{Corr}[Y]$, from $\text{Cov}[Y]$.
 5. Apply the vector of standard deviations, $\sqrt{\Sigma_{ii}}$, to $\text{Corr}[Y]$ to obtain the off-diagonal elements of Σ .
 6. Sample from the multivariate normal distribution defined by μ and Σ .
 7. Exponentiate the samples.
 8. Restore components in the samples that were deleted because of zero variance.
 9. Impose the constraints on each sample.
- Up until the last step, the means and standard deviations of the samples are the same as originally specified. Only the covariances are different.
 - This works well for our case (means and standard deviations of the samples are almost unchanged and covariances are close) but there is no guarantee that this will be true in other cases.

Sampling and Fitting to Jezebel

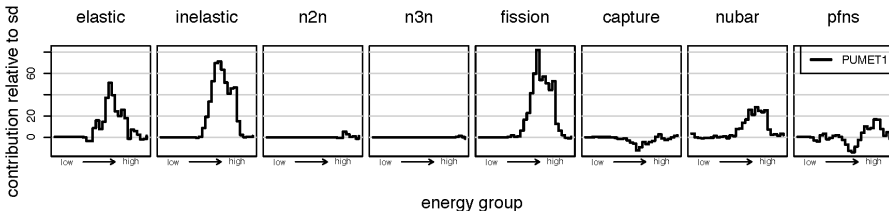
- Sample from cross sections, $\bar{\nu}$, and the PFNS independently and composite the samples.
- Discard any composite samples that have negative cross sections.
- Produce Nuclear Data Interface (NDI) tables for the surviving samples.
- Use the NDI tables as the ^{239}Pu data for simulations of Jezebel, computing k-effective.
- Do sensitivity analysis to understand which inputs play a significant role in k-effective.
 - We used a regularized version of sliced inverse regression (SIR) with hold-some-back cross validation to identify the dominant modes in the nuclear data.
- Weight each sample by the likelihood of its value of k-effective.
 - The weighted samples are a representation of the posterior distribution for the nuclear data, after taking the Jezebel results into account.
- Analyze the posterior by, for example, computing the weighted sample mean vector and covariance matrix.

Sensitivities I



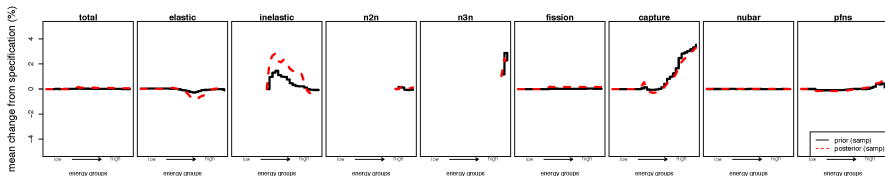
- Each color shows the mean, divided by the corresponding standard deviation, of the samples in a particular quantile of the $k_{\text{effective}}$ space.
 - For example, the deep green shows the mean of the samples that produce the lowest 5% of the $k_{\text{effective}}$ values.
- The plot makes it possible to see which nuclear data play a significant role in determining $k_{\text{effective}}$, and how they trade off against each other.
 - Fission obviously plays the biggest role.
 - The lowest quantile corresponds to low values for the fission cross section, $\bar{\nu}$, and inelastic scattering, high values for elastic scattering and capture, and a softening of the PFNS (decreased values at high energies and increased values at low energies), as expected.

Sensitivities II



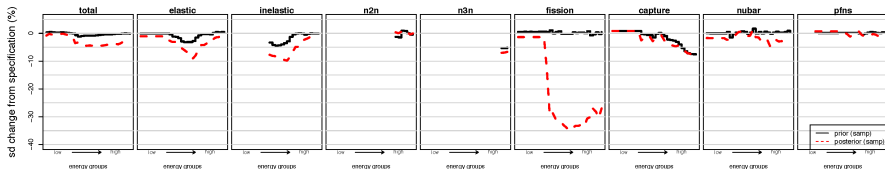
- There is a single mode of variation for the nuclear data that completely dominates k-effective.
- The response to this model of variation is linear.
- For any set of nuclear data, the dot product with this mode is what determines k-effective.
- This is still true after we do the fit to Jezebel.

Sampling and Fitting: Means



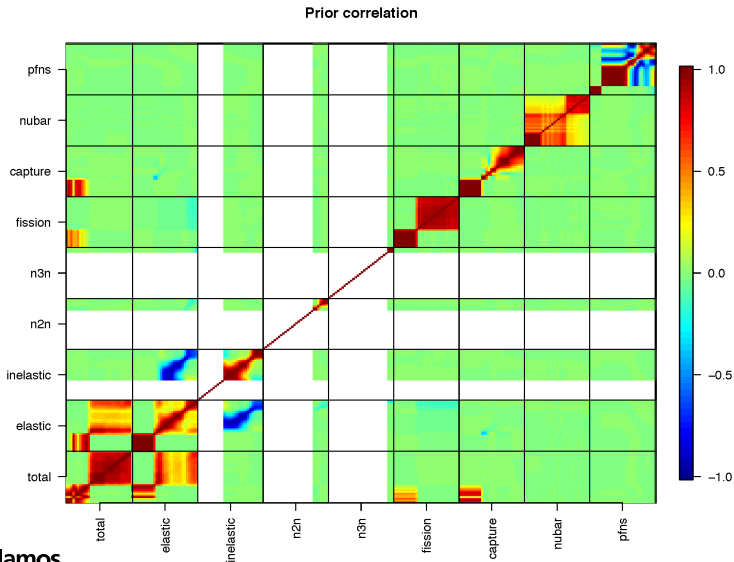
- Black shows changes in the means due to sampling error and tossing out negative cross sections.
 - The changes occur where we expect them to, in the data that have large relative standard deviations.
 - The biggest changes, for high-energy capture and n3n, are under 4%. The others are much smaller.
- Red shows changes in the means due to fitting to Jezebel.
 - The only effect of fitting on the means is on the inelastic scattering, which increases modestly.

Sampling and Fitting: Standard Deviations

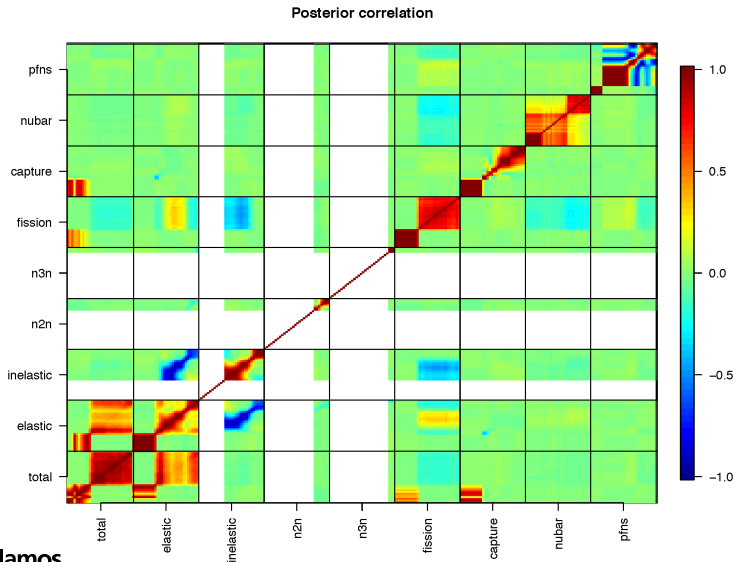


- Black shows changes in the standard deviations due to sampling error and tossing out negative cross sections.
 - The changes are quite small except for high energy capture, which decreases by about 8%.
- Red shows changes in the standard deviations due to fitting to Jezebel.
 - The effects are substantial. Fission decreases by almost 35%. Elastic and inelastic scattering decrease by up to 10% and total scattering decreases by about 5%.

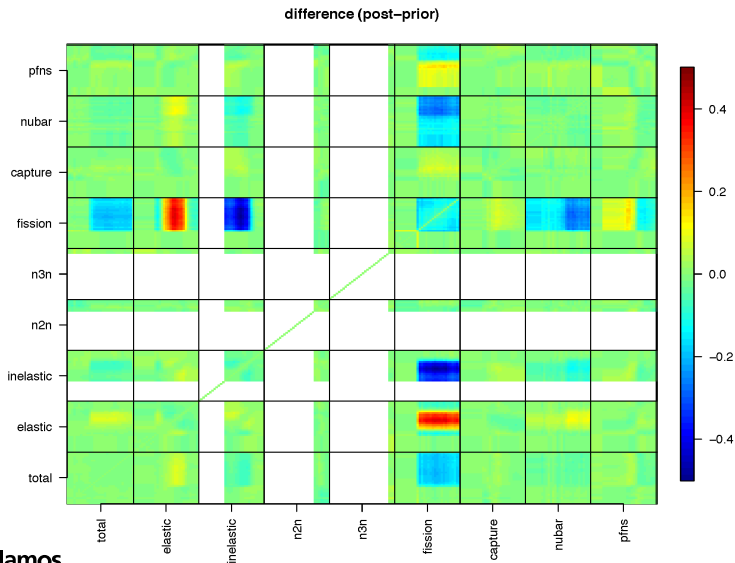
Prior Correlations



Posterior Correlations



Changes in Correlations



The Effects of Fitting on Correlations

- Reduced positive correlations among the fission values, allowing them to trade off against each other.
- Negative correlations between fission and $\bar{\nu}$.
- Negative correlations between fission and hardening of the PFNS.
- Other effects are more complex:
 - Negative correlations between fission and inelastic scattering.
 - Positive correlation between fission and elastic scattering.
- In general, the fitted correlations give us **a quantitative picture of compensating errors.**